

Hypergraph Automata: A Theoretical Model for Patterned Self-assembly

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Abstract. Patterned self-assembly is a process whereby coloured tiles self-assemble to build a rectangular coloured pattern. We propose *self-assembly (SA) hypergraph automata* as an automata-theoretic model for patterned self-assembly. We investigate the computational power of SA-hypergraph automata and show that for every recognizable picture language, there exists an SA-hypergraph automaton that accepts this language. Conversely, we prove that for any restricted SA-hypergraph automaton, there exists a Wang Tile System, a model for recognizable picture languages, that accepts the same language. The advantage of SA-hypergraph automata over Wang automata, acceptors for the class of recognizable picture languages, is that they do not rely on an *a priori* defined scanning strategy.

1 Introduction

DNA-based self-assembly is an autonomous process whereby a disordered system of DNA sequences forms an organized structure or pattern as a consequence of Watson-Crick complementarity of DNA sequences, without external direction. A DNA-tile-based self-assembly system starts from DNA “tiles”, each of which is formed beforehand from carefully designed single-stranded DNA sequences which bind via Watson-Crick complementarity and ensure the tiles’ shape (square) and structure. In particular, the sides and interior of the square are double-stranded DNA sequence, while the corners have protruding DNA single strands that act as “sticky ends”. Subsequently, the individual tiles are mixed together and interact locally via their sticky-ends to form DNA-based *supertiles* whose structure is dictated by the base-composition of the individual tiles’ sticky ends. Winfree [15] introduced the abstract Tile Assembly Model (aTAM) as a mathematical model for tile-based self-assembly systems. Ma [13] introduced the patterned self-assembly of single patterns, whereby coloured tiles self-assemble to build a particular rectangular *coloured pattern*. Patterned self-assembly models a particular type of application in which tiles may differ from each other by some distinguishable properties, modelled as colours [14,2]. Orponen [7,10] designed several algorithms to find the minimum tile set required to construct one given coloured pattern. Czeizler [4] proved that this minimization problem is NP-hard.

In this paper, we propose *self-assembly (SA) hypergraph automata* as a general model for patterned self-assembly and investigate its connections to other models for two-dimensional information and computation, such as 2D (picture) languages and Wang Tile Systems. A 2D (picture) language consists of 2D words (pictures), defined as mappings $p : [m] \times [n] \rightarrow [k]$ from the points in the two-dimensional space to a finite alphabet of cardinality k . Here, $[k]$ denotes the set $[k] = \{1, 2, \dots, k\}$. Note that, if we take the alphabet $[k]$ to be a set of colours, the definition of a picture is analogous to that of a coloured pattern [13].

Early generating/accepting systems for 2D languages comprise 2×2 tiles [6], 2D automata [3], two-dimensional on-line tessellation acceptors [8], and 2D grammars. More recently a generating system was introduced by Varricchio [5] that used *Wang tiles*. A *Wang tile system* [5] is a specialized tile-based model that generates the class of *recognizable picture languages*, a subclass of the family of 2D languages. The class of recognizable picture languages is also accepted by *Wang automata*, a model introduced in [11]. Like other automata for 2D languages [1], Wang tile automata use an explicit pre-defined scanning strategy [12] when reading the input picture and the accepted language depends on the scanning strategy that is used. Due to this, Wang automata are a suboptimal model for self-assembly. Indeed, if we consider the final supertile as given, the order in which tiles are read is irrelevant. On the other hand, if we consider the self-assembly process which results in the final supertile, an “order of assembly” cannot be pre-imposed. In contrast to Wang automata, SA-hypergraph automata are scanning-strategy-independent.

SA-hypergraph automata are a modification of the hypergraph automata introduced by Rozenberg [9] in 1982. An SA-hypergraph automaton (Section ??) accepts a language of labelled “rectangular grid graphs”, wherein the labels are meant to capture the notion of colours used in patterned self-assembly. An SA-hypergraph automaton consists of an underlying labelled graph (labelled nodes and edges) and a set of *hyperedges*, each of which is a subset of the set of nodes of the underlying graph. Intuitively, the hyperedges are meant to model tiles or supertiles while the underlying graph describes how these can attach to each other, similar to a self-assembly process.

We investigate the computational power of SA-hypergraph automata and prove that for every recognizable picture language L there is an SA-hypergraph automaton that accepts L (Thm. 1). Moreover, we prove that for any restricted SA-hypergraph automaton, there exists a Wang tile system that accepts the same language of coloured patterns (Thm. 2). Here, restricted SA-hypergraph automaton means an SA-hypergraph automaton in which certain situations that cannot occur during self-assembly are explicitly excluded.

2 Preliminaries

A picture (two-dimensional word) p over the alphabet Σ is a two dimensional matrix of letters from Σ . Each element of this matrix is called a pixel. $p_{(i,j)}$ denotes the pixel in the i th row and j th column of this matrix. Two pixels $p_{(i,j)}$

and $p_{(i',j')}$ are adjacent if $|i - i'| + |j - j'| = 1$. The function $w(p)$ denotes the width and $h(p)$ denotes the height of the picture p . Σ^{**} is the set of all pictures over the alphabet Σ . Let $\#$ be a letter which does not belong to the alphabet Σ . The *framed picture* \hat{p} of $p \in \Sigma^{**}$ is defined as:

$$\hat{p} = \begin{array}{ccccc} \# & \# & \cdots & \# & \# \\ \# & p_{(1,1)} & \cdots & p_{(1,w(p))} & \# \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \# & p_{(h(p),1)} & \cdots & p_{(h(p),w(p))} & \# \\ \# & \# & \cdots & \# & \# \end{array}$$

A *picture language* (2D language) is a set of pictures over an alphabet Σ . For example, $L = \{p \in \Sigma^{**} \mid \text{for all } 1 \leq i \leq h(p), p_{(i,1)} = p_{(i,w(p))}\}$ is the language of all rectangles that have the same first and last column.

A function $\delta: \mathbb{N}^2 \rightarrow \mathbb{N}^2$ is a *translation function* if there exists $i', j' \in \mathbb{Z}$ such that $\delta(i, j) = (i + i', j + j')$ for all $i, j \in \mathbb{N}$. A *subpicture* over Σ is a two-dimensional matrix of letters from $\Sigma \cup \{\text{empty}\}$. A subpicture q is *connected* if for every pair of pixels $q_{(i',j')}, q_{(i,j)} \in \Sigma$ there exists a sequence of pixels $s = \langle s_0, s_1, \dots, s_n \rangle$ from q such that $s_0 = q_{(i,j)}$ and $s_n = q_{(i',j')}$, for all $0 \leq k < n$, we have $s_k \in \Sigma$. Moreover, s_k and s_{k+1} must be adjacent. If p is a picture, then q is a subpicture of p if there exists a translation function δ such that for all $(i, j) \in [h(q)] \times [w(q)]$ we have either $q_{(i,j)} = \text{empty}$ or $q_{(i,j)} = p_{\delta(i,j)}$.

A *picture tile* is a 2×2 picture (for example $\begin{bmatrix} a & b \\ c & d \end{bmatrix}$). The language defined by a set of picture tiles Δ over the alphabet $\Sigma \cup \{\#\}$ is denoted by $\mathcal{L}(\Delta)$ and is defined as the set of all pictures $p \in \Sigma^{**}$ such that any 2×2 subpicture of \hat{p} is in Δ . Giammarresi [6] defined a *Picture Tiling System* (PTS) as a 4-tuple $T = (\Sigma, \Gamma, \Delta, \pi)$, where Σ and Γ are two finite alphabets, Δ is a finite set of picture tiles over $\Gamma \cup \{\#\}$ and $\pi: \Gamma \rightarrow \Sigma$ is a projection. The PTS T recognizes the language $\mathcal{L}(T) = \pi(\mathcal{L}(\Delta))$. A picture language L is called *PTS-recognizable* if there exists a picture tiling system T such that $L = \mathcal{L}(T)$. Figure 1 shows an example.

A equivalent definition of recognizability was proposed using labelled Wang tiles [12]. A labelled Wang tile, shortly LWT, is a labelled unit square whose edges may be coloured. Formally, a LWT is a 5-tuple (c_N, c_E, c_S, c_W, l) , where l belongs to a finite set of labels Σ and c_N, c_E, c_S , and c_W belong to $C \cup \{\#\}$ where C is a finite set of colours and $\#$ represents an uncoloured edge. Intuitively, c_N, c_E, c_S , and c_W represent the colour of the north, east, south, and west edge of the tile, respectively. Labelled Wang tiles cannot rotate. The colours on the north, south, east, and west edges of an LWT t are denoted by $\sigma_N(t)$, $\sigma_S(t)$, $\sigma_E(t)$, and $\sigma_W(t)$, respectively; moreover, $\lambda(t)$ denotes the label of t .

A Wang Tile System (WTS)[5] is a triple $W = (\Sigma, C, \Theta)$ where Σ and C are two finite alphabets (the alphabet of tile labels and the alphabet of colours,

i)

#	#	1	#	#	0	#	#
#	1	#	#	#	#	0	#
#	#	#	#	0	0	0	1
1	0	0	0	#	#	#	#
#	0	#	1	0	#	0	#
#	0	#	0	0	#	1	#
1	0	0	0	0	1	0	0
0	1	0	0	0	0	1	0

ii)

#	#	#	#	#	#
#	1	0	0	0	#
#	0	1	0	0	#
#	0	0	1	0	#
#	0	0	0	1	#
#	#	#	#	#	#

iii)

#	#	#	#	#	#
#	a	a	a	a	#
#	a	a	a	a	#
#	a	a	a	a	#
#	a	a	a	a	#
#	#	#	#	#	#

Fig. 1. Let $T = (\Sigma, T, \Delta, \pi)$ be the picture tile system where $\Sigma = \{a\}$, $\Gamma = \{0, 1\}$, $\pi(0) = \pi(1) = a$ and Δ consists of the 16 different picture tiles in i). The PTS T recognizes the language containing all square pictures p where $w(p) = h(p) \geq 2$ and where every pixel is labelled with a . Part ii) is an example of framed picture \hat{p} in $\mathcal{L}(\Delta)$, and iii) shows the projection $\pi(\hat{p})$ of the framed picture in part ii).

respectively) with $\# \notin C$, and Θ is a finite set of labelled Wang tiles with labels from Σ and colours from C . The WTS W recognizes the picture language $\mathcal{L}(W)$ where the picture $p \in \Sigma^{**}$ belongs to $\mathcal{L}(W)$ if and only if there exists a mapping $m: [h(p)] \times [w(p)]$ from the pixels of p to tiles from Θ such that the label of the tile $m(p_{(i,j)})$ is equal to $p_{(i,j)}$; moreover, this mapping must be *mismatch free*. The mapping m is mismatch free if for two adjacent pixels $p_{(i,j)}$ and $p_{(i+1,j)}$ in p the south edge of $m(p_{(i,j)})$ and the north edge of $m(p_{(i+1,j)})$ are coloured by the same colour from C ; for two adjacent pixels $p_{(i,j)}$ and $p_{(i,j+1)}$ in p the east edge of $m(p_{(i,j)})$ and the west edge of $m(p_{(i,j+1)})$ are coloured by the same colour from C ; and for every border pixel $p_{(i,j)}$ with $i = 1$, $j = 1$, $i = h(p)$, or $j = w(p)$ we require that the north, west, south, or east edge, respectively, of $m(p_{(i,j)})$ is uncoloured. For a pixel in a corner, e.g. $p_{(1,1)}$, this implies that two edges are uncoloured. Let \bar{p} be a two dimensional array of labelled Wang tiles from Θ . We call \bar{p} a Wang tiled version of the picture p if the width and the height of p and \bar{p} are equal, and there exists a mismatch free mapping m such that for any i and j we have $\bar{p}_{(i,j)} = m(p_{(i,j)})$. Two tiles $\bar{p}_{(i,j)}$ and $\bar{p}_{(i',j')}$ are adjacent if the pixels $p_{(i,j)}$ and $p_{(i',j')}$ are adjacent. A language L is *WTS-recognizable* if there exists a Wang tile system W such that W recognizes L . Figure 2 shows an example.

Proposition 1 ([6]). *A picture language L is PTS-recognizable if and only if it is WTS-recognizable.*

A coloured pattern, as defined in [13] is the end result of a self-assembly process that starts with a fixed-size L -shaped seed supertile and proceeds as in Figure 3, (i), until one coloured rectangle is formed. Note that Wang Tile Systems can be seen as generating (potentially infinite) languages of such coloured patterns where the L -shaped seed is of an arbitrary size and is generated starting from a single-tiled seed with uncoloured North and West edges, and is extended by tiles with uncoloured North or West edges, as shown in Figure 3, (ii).

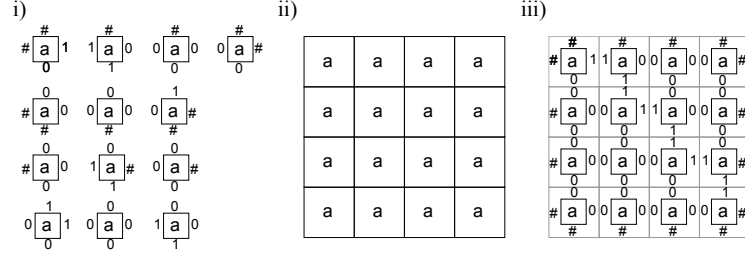


Fig. 2. Let $W = (\Sigma, C, \Theta)$ be the Wang Tile System where $\Sigma = \{a\}$, $C = \{0, 1\}$ and Θ consists of the 13 LWTs shown in i). This Wang tile system recognizes the picture language containing all square pictures p with $h(p) = w(p) \geq 3$ and where every pixel is labelled by a . Part ii) is an example picture and iii) shows the Wang tiled version of the picture in part ii).

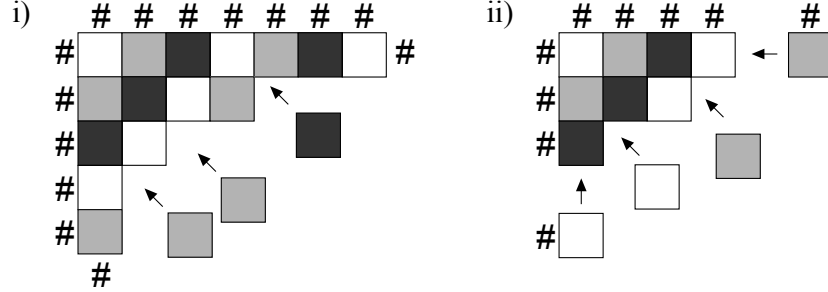


Fig. 3. (i) The self-assembly of a single *coloured pattern*, starting with a fixed-size *L*-shaped seed. (ii) The process of generating a *picture* in the language of a *Wang Tile System*.

3 Hypergraph Automata

Let $f: A \rightarrow B$ be a function and let $A' \subseteq A$. The *restriction* of f to A' is $f|_{A'}: A' \rightarrow B$ such that $f|_{A'}(x) = f(x)$ for all $x \in A'$. For any set A we let $id_A: A \rightarrow A$ denote the *identity*. When the set A is clear from the context, we will omit the subscript and simply write id .

Let Σ be an alphabet. A *pseudo-picture graph* is a directed labelled graph $G = (N, E_v \cup E_h, \pi)$ where N is a finite set of nodes, $E_v, E_h \subseteq N \times N$ are two sets of edges such that $E_v \cap E_h = \emptyset$, and $\pi: N \rightarrow \Sigma$ is the label function. Edges from E_v and E_h will frequently be denoted by \xrightarrow{v} and \xrightarrow{h} , respectively. The *node-induced subgraph* of G by a subset $N' \subseteq N$ is defined as the graph $(N', E'_v \cup E'_h, \pi|_{N'})$ where $E'_v = \{(x, y) \in E_v \mid x, y \in N'\}$ and $E'_h = \{(x, y) \in E_h \mid x, y \in N'\}$. A graph G' is called a *full subgraph* of G if for some $N' \subseteq N$ it is the node-induced subgraph of G by N' .

A pseudo-picture graph $G = (N, E_v \cup E_h, \pi)$ is an $(n \times m)$ -picture graph (for $n, m \in \mathbb{N}$) if there is a bijection $f_G: N \rightarrow [N] \times [M]$ such that for $x, y \in N$, we have $(x, y) \in E_v$ if and only if $f_G(x) + (1, 0) = f_G(y)$, and $(x, y) \in E_h$ if and only if $f_G(x) + (0, 1) = f_G(y)$. We want to stress that we do not use Cartesian coordinates; our pictures are defined as matrices, hence, incrementing the first coordinate corresponds to a step downwards, and incrementing the second coordinate corresponds to a step rightwards. In other words, the nodes of a picture graph G can be embedded in \mathbb{N}^2 such that every edge in E_v has length 1 and points downwards, every edge in E_h has length 1 and points rightwards, and every two nodes with Euclidean distance 1 are connected by an edge. Note that if a pseudo-picture graph is an $n \times m$ -picture graph, it cannot be an $n' \times m'$ -picture graph with $n \neq n'$ or $m \neq m'$, and the function f_G is unique. If G is a picture graph, we call $e \in E_v$ a *vertical edge* and $e \in E_h$ a *horizontal edge*. The set of all picture graphs is denoted by \mathcal{G} . Every $n \times m$ -picture graph $G = (N, E_v \cup E_h, \pi)$ represents a picture $p(G) \in \Sigma^{**}$ with $h(p(G)) = n$ and $w(p(G)) = m$. More precisely, for all $(i, j) \in [n] \times [m]$ we let $p(G)_{(i,j)} = \pi(f_G^{-1}(i, j))$. Hence, $p: \mathcal{G} \rightarrow \Sigma^{**}$ can be seen as a function.

A connected pseudo-picture graph G is called a *subgrid* if it is a full subgraph of a picture graph G' . We also say G is a subgrid of G' .

A *hypergraph* [9] is a triple $H = (N, E, f)$ where N is the finite set of nodes, E is the finite set of *hyperedges*, and $f: E \rightarrow \mathcal{P}(N)$ is a function assigning to each hyperedge a set of nodes; the same set of nodes may be assigned to two distinct hyperedges. For every hyperedge $e \in E$, we let

$$I_H(e) = \{x \in N \mid \exists e' \in E \setminus \{e\}: x \in f(e) \cap f(e')\}$$

be the set of *intersecting nodes* in $f(e)$. Rozenberg [9] introduced *hypergraph automata* to describe graph languages. Here, we modified Rozenberg's definition in order to study pseudo-picture graphs. Figure 4 shows an one dimensional example of an automaton based on a hypergraph. The formal definition is as follows.

Definition 1. A self-assembly (SA) hypergraph automaton is a tuple $A = (N, E, f, d, G, E_0)$ where $H = (N, E, f)$ is a hypergraph, called the underlying hypergraph, $d: E \rightarrow I_H(e) \times I_H(e)$ is the transition function assigning to each hyperedge $e \in E$ a transition $Q_1 \rightarrow Q_2$ with $Q_1, Q_2 \subseteq I_H(e)$, G is a pseudo-picture graph with node set N called the underlying graph, and $E_0 \subseteq E$ is the set of initial hyperedges.

Every hyperedge $e \in E$ defines a graph G_e which is the subgraph of G induced by $f(e)$. For $d(e) = Q_1 \rightarrow Q_2$ we call Q_1 and Q_2 the *incoming active nodes* and *outgoing active nodes* of G_e , respectively. In order for the hypergraph automaton to be well-defined, we require that G_e is connected and that the subgraph of G_e induced by its incoming active nodes is connected, too, for all $e \in E$. If $e \in E_0$, then G_e is also called an *initial graph*.

A *configuration* of the hypergraph automaton A is a triple (M, O, g) where $M = (N_M, E_{M,v} \cup E_{M,h}, \pi_M)$ is a subgrid, $O \subseteq N_M$ is the set of *active nodes*,

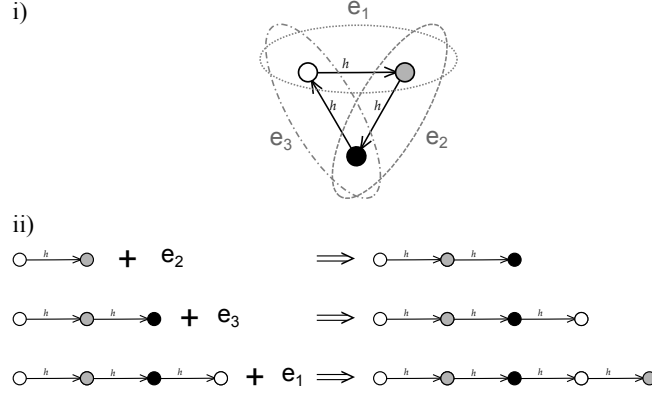


Fig. 4. The hypergraph in part i) consists of three hyperedges. Intuitively, a derivation of the hypergraph automaton starts from the initial hyperedge e_1 and in each step adds the underlying graph of another hyperedge to the current configuration. In part ii) we start with the hyperedge e_1 , afterwards, the underlying graph of the hyperedge e_2 is added to the current configuration. In the next step, the underlying graph of hyperedge e_3 is added. In the last step, the hyperedge e_1 is reused. Repeating this process, an arbitrary long chain of nodes, forming a white-grey-black pattern, can be constructed using only the three hyperedges.

and $g: N_M \rightarrow N$ is a function such that $\pi_M(x) = \pi(g(x))$ for all $x \in N_M$. The set N_M consists of (possibly multiple) copies of nodes from N and the function g assigns to each node in N_M its original node in N . An edge $(x, y) \in E_{M,h}$ is a copy of the edge $(g(x), g(y)) \in E_h$ and $(x, y) \in E_{M,v}$ is a copy of the edge $(g(x), g(y)) \in E_v$. However, for two nodes x and y in M , if their originals $g(x)$ and $g(y)$ are connected by a horizontal (or vertical) edge, this does not imply that x and y are connected by a horizontal (or vertical) edge.

Let (M_1, O_1, g_1) be a configuration with $M_1 = (N_1, E_{1,v} \cup E_{1,h}, \pi_1)$ and let $e \in E$ be a hyperedge with $d(e) = Q_1 \rightarrow Q_2$. If there exists a non-empty subset $P \subseteq O_1$ such that $g_1|_P$ forms a graph-isomorphism from the subgraph of M_1 induced by P to the subgraph of G_e induced by the incoming active nodes Q_1 , then the hyperedge e defines a *transition* or *derivation step*

$$(M_1, O_1, g_1) \xrightarrow{A} (M_2, O_2, g_2)$$

where, informally speaking, the resulting graph M_2 consists of joining together the graphs M_1 and G_e by identifying every node $x \in P$ with the corresponding node $g_1(x) \in Q_1$. The active nodes O_2 in M_2 are the active nodes $O_1 \setminus P$ in M_1 plus the outgoing active nodes Q_2 in G_e , see Figure 5. We also say that (M_2, O_2, g_2) is the result of *gluing* the hyperedge e to (M_1, O_1, g_1) . Formally, the configuration (M_2, O_2, g_2) where $M_2 = (N_2, E_{2,v} \cup E_{2,h}, \pi_2)$ is constructed as follows. Let $N' = \{x' \mid x \in f(e) \setminus Q_1\}$ be a set containing a copy of each node from G_e except for the incoming active nodes such that $N' \cap N_1 = \emptyset$.

Let $N_2 = N_1 \cup N'$ and let $g_2: N_2 \rightarrow N$ such that $g_2(x) = g_1(x)$ for $x \in N_1$ and $g_2(x') = x$ for $x' \in N'$. An edge (x, y) belongs to $E_{2,v}$ if $(x, y) \in E_{1,v}$ or $x, y \in P \cup N'$ and $(g(x), g(y)) \in E_v$; an edge (x, y) belongs to $E_{2,h}$ if $(x, y) \in E_{1,h}$ or $x, y \in P \cup N'$ and $(g(x), g(y)) \in E_h$. Naturally, $\pi_2(x) = \pi(g_2(x))$ for all $x \in N_2$ and $O_2 = (O_1 \setminus P) \cup \{x' \in N' \mid x \in Q_2\}$. The reflexive and transitive closure of $\xrightarrow[A]{}$ is denoted by $\xrightarrow[A]{*}$ and called a *derivation*.

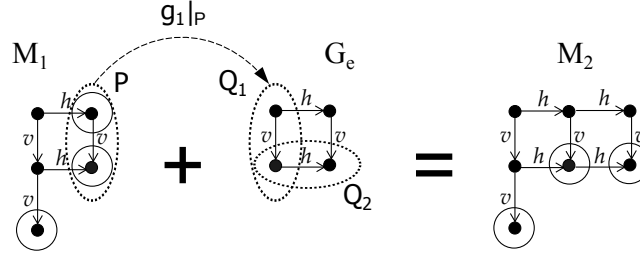


Fig. 5. A transition $(M_1, O_1, q_1) \rightarrow_A (M_2, O_2, q_2)$ joins together the graphs M_1 and G_e by identifying every node $x \in P$ with the corresponding node $g_1(x) \in Q_1$. The set O_2 of the active nodes of the new configuration M_2 consists of the nodes of the union of the active nodes in $O_1 \setminus P$ with the outgoing active nodes Q_2 of G_e . The active nodes of M_1 and M_2 are represented as circled nodes.

For $e \in E_0$ we let O_e such that $d(e) = Q_1 \rightarrow O_e$ and we call the configuration (G_e, O_e, id) an *initial configuration* of A . A *final configuration* is a configuration (M, \emptyset, g) without active nodes. The graph language accepted by the SA-hypergraph automaton A is

$$\mathcal{L}(A) = \left\{ M \in \mathcal{G} \mid \exists e \in E_0: (G_e, O_e, id) \xrightarrow[A]{*} (M, \emptyset, g) \right\}.$$

Note that $\mathcal{L}(A)$ contains picture graphs only. The *picture language associated to the graph language $\mathcal{L}(A)$* is the language $p(\mathcal{L}(A))$.

Remark 1. Since we only talk about picture graphs, we can assume that for every hyperedge $e \in E$ the underlying graph G_e is a subgrid, or e can be removed from the set E .

Example 1. Figure 6 shows an example of a self-assembled coloured pattern and an SA-hypergraph automaton that accepts that pattern. Part i) depicts a coloured self-assembled pattern. Parts ii) and iii) together depict the underlying graph of the SA-hypergraph automaton that constructs the same pattern.

The SA-hypergraph automaton for the example in Figure 5 is defined as follows. The SA-hypergraph automaton is $A = (N, E, f, d, G, E_0)$, where

- $N = \{x_1, x_2, \dots, x_9, z_1, z_2, \dots, z_7\}$,

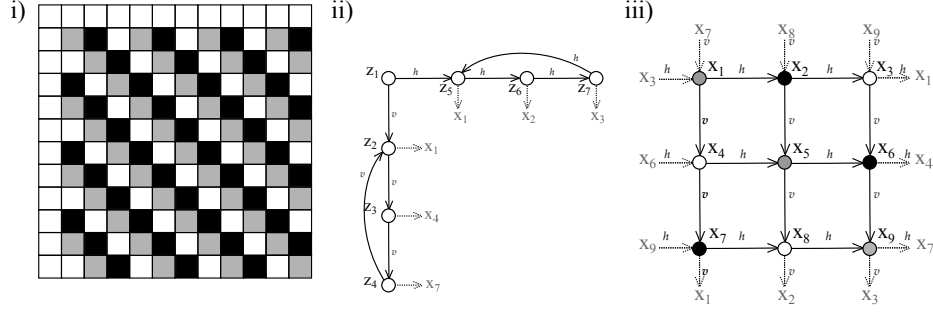


Fig. 6. Part i) shows an example of coloured self-assembled pattern. Parts ii) and iii) together depict the underlying graph of the SA-hypergraph automaton that constructs the same pattern. Part ii) constructs the white top row and white left column, and part iii) constructs the coloured pattern.

- $E = \{e_1, e_2, \dots, e_{16}\}$,
- function f is defined such that

$$\begin{aligned}
 f(e_1) &= \{x_1, x_2, x_4, x_5\}, & f(e_2) &= \{x_2, x_3, x_5, x_6\}, & f(e_3) &= \{x_3, x_1, x_6, x_4\}, \\
 f(e_4) &= \{x_4, x_5, x_7, x_8\}, & f(e_5) &= \{x_5, x_6, x_8, x_9\}, & f(e_6) &= \{x_6, x_4, x_9, x_7\}, \\
 f(e_7) &= \{x_7, x_8, x_1, x_2\}, & f(e_8) &= \{x_8, x_9, x_2, x_3\}, & f(e_9) &= \{x_9, x_7, x_3, x_1\}, \\
 f(e_{10}) &= \{z_1, z_5, z_2, x_1\}, & f(e_{11}) &= \{z_5, z_6, x_1, x_2\}, & f(e_{12}) &= \{z_6, z_7, x_2, x_3\}, \\
 f(e_{13}) &= \{z_7, z_5, x_3, x_1\}, & f(e_{14}) &= \{z_2, x_1, z_3, x_4\}, & f(e_{15}) &= \{z_3, x_4, z_4, x_7\}, \\
 f(e_{16}) &= \{z_4, x_7, z_2, x_1\}.
 \end{aligned}$$

- For each hyperedge in ii), the function d describing the active areas where we can glue new hyperedges is defined as to build a horizontal (vertical) chain of nodes that models the top row (left column) of tiles.

$$\begin{aligned}
 d(e_{11}) &= \{z_5, x_1\} \rightarrow \{z_6, x_1, x_2\}, & d(e_{12}) &= \{z_6, x_2\} \rightarrow \{z_7, x_2, x_3\}, \\
 d(e_{13}) &= \{z_7, x_3\} \rightarrow \{z_5, x_1, x_3\}, & d(e_{14}) &= \{z_2, x_1\} \rightarrow \{z_3, x_1, x_4\}, \\
 d(e_{15}) &= \{z_3, x_4\} \rightarrow \{z_4, x_4, x_7\}, & d(e_{16}) &= \{x_7, z_4\} \rightarrow \{z_2, x_1, x_2\}.
 \end{aligned}$$

The backward edges e.g. (x_3, x_1) , (x_4, x_6) , (x_7, x_9) , and (z_7, z_5) , make it possible to reuse the hyperedges to build a periodic pattern.

For each hyperedge in iii), the function d changes the active input nodes (top-left, bottom-left, and top-right) to the new set of active nodes (top-right, bottom-left, and bottom-right), signifying the change of the places where the new hyperedges can be glued.

$$\begin{aligned}
d(e_1) &= \{x_1, x_2, x_4\} \rightarrow \{x_2, x_4, x_5\}, & d(e_2) &= \{x_2, x_3, x_5\} \rightarrow \{x_3, x_5, x_6\}, \\
d(e_3) &= \{x_3, x_1, x_4\} \rightarrow \{x_1, x_6, x_4\}, & d(e_4) &= \{x_4, x_5, x_7\} \rightarrow \{x_5, x_7, x_8\}, \\
d(e_5) &= \{x_5, x_6, x_8\} \rightarrow \{x_6, x_8, x_9\}, & d(e_6) &= \{x_6, x_4, x_9\} \rightarrow \{x_4, x_9, x_7\}, \\
d(e_7) &= \{x_7, x_8, x_1\} \rightarrow \{x_8, x_1, x_2\}, & d(e_8) &= \{x_8, x_9, x_2\} \rightarrow \{x_9, x_2, x_3\}, \\
d(e_9) &= \{x_9, x_7, x_3\} \rightarrow \{x_7, x_3, x_1\}, & d(e_{10}) &= \{z_1, z_5, z_2\} \rightarrow \{z_5, x_1, z_2\}.
\end{aligned}$$

- Parts ii) and iii) depict the underlying graphs of the white Γ -shaped top and left border of the pattern, and the white-grey-black part of the pattern respectively.
- $E_0 = \{e_{10}\}$

The SA-hypergraph automaton A starts from the top-left white tile, corresponding to $E_0 = \{e_{10}\}$. Afterwards, the automaton continues the construction with the hyperedges in the top row or the left column. The construction of the white-grey-black part starts after the construction of the white top row and left column. Figure 7 shows an example of possible transitions of the SA-hypergraph automaton A .

The concept of hypergraph automata has been introduced by Rozenberg in 1982 [9]. Our definition of SA-hypergraph automata is a variant of the original definition with the following modifications. Firstly, we start from a set of initial graphs whereas the original definition used a single initial graph. For unlabelled graphs both models are capable of accepting the same class of graph languages, as long as one makes an exception for the empty graph. However, for labelled graphs a single initial graph is not sufficient; e.g., if a language L of labelled graphs contains one graph A where every node is labelled by a and one graph B where every node is labelled by b , then L cannot be generated from the same initial graph since A and B do not have a common non-empty isomorphic subgraph. Secondly, we use final configurations in order to accept only some of the graphs that can be generated by rules from the initial graph. In the original definition, for simplicity, final configurations were omitted and every graph which can be generated from the initial graph belonged to the accepted language. Thirdly, it seemed more convenient to us to use the notion of active nodes rather than active intersections.

4 Some Examples

In this section, we provide three example SA-hypergraph automata and illustrate their relation to self-assembly systems. Our findings, presented in Section 5, do not build upon this section. In all examples, every node in the underlying graph has a distinct colour which, for simplicity, is the same as the identifier of the node.

The following examples shows a SA-hypergraph automaton to accept the pictures in Figure 8 part a). This example shows that SA-hypergraph automata

- function d is defined such that

$$d(e_1) = \{x_1, x_2\} \rightarrow \{x_3, x_4\},$$

$$d(e_2) = \{x_3, x_4\} \rightarrow \{\},$$

$$d(e_3) = \{x_3, x_4\} \rightarrow \{\}$$

- underlying graph is shown in Figure 8 part b.
- $E_0 = \{e_1\}$

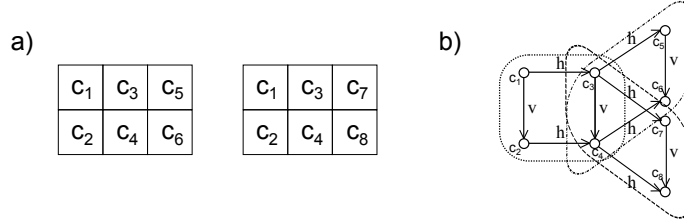


Fig. 8. Part a) shows an example of language of coloured self-assembled patterns. Parts b) depicts the underlying graph of the SA-hypergraph automaton that constructs the same pattern.

Example 3 shows a simple picture language containing two 2D-words. The SA-hypergraph automaton uses two overlapping hyperedges with different active inputs and outputs. Therefore, the number of nodes in this SA-hypergraph automaton will be less than the number tiles in a tile assembly system which recognizes the same language. The SA-hypergraph automaton in this example has 4 nodes and 3 hyperedges. An equivalent tile assembly system needs at least 6 tile types.

Example 3. The SA-hypergraph automaton for the example in Figure 9 is defined as follows. The SA-hypergraph automaton is $A = (N, E, f, d, G, E_0)$, where

- $N = \{x_1, x_2, x_3, x_4\}$,
- $E = \{e_1, e_2, e_3\}$,
- function f is defined such that

$$f(e_1) = \{x_1, x_2\},$$

$$f(e_2) = \{x_1, x_2\},$$

$$f(e_3) = \{x_1, x_2, x_3, x_4\}$$

- function d is defined such that

$$d(e_1) = \{x_1\} \rightarrow \{\},$$

$$d(e_2) = \{x_1\} \rightarrow \{x_1, x_2\},$$

$$d(e_3) = \{x_1, x_2\} \rightarrow \{\}$$

- underlying graph is shown in Figure 9 part b).
- $E_0 = \{e_1, e_2\}$

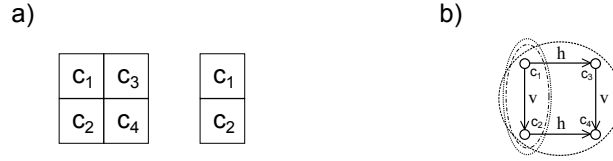


Fig. 9. Part a) shows an example of language of coloured self-assembled patterns. Parts b) depicts the underlying graph of the SA-hypergraph automaton that constructs the same pattern.

Example 4 shows a language with an infinite number of one dimensional pictures. The SA-hypergraph automaton uses three hyperedges to build the chain, moreover, one more hyperedge is used to make the final configurations. Therefore, the number of nodes in this SA-hypergraph automaton will be less than the number tiles in a tile assembly system which recognizes the same language. The SA-hypergraph automaton in this example has 3 nodes and 4 hyperedges. Whereas an equivalent tile assembly system needs at least 5 tile types (one tile type to start, 3 tile type to build the chain, and one tile type to stop).

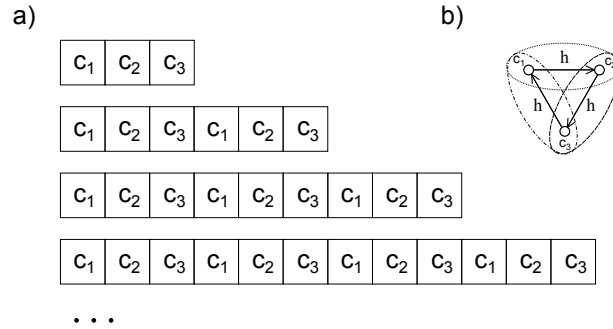


Fig. 10. Part a) shows an example of language of coloured self-assembled patterns. Parts b) depicts the underlying graph of the SA-hypergraph automaton that constructs the same pattern.

Example 4. The SA-hypergraph automaton for the example in Figure 10 is defined as follows. The SA-hypergraph automaton is $A = (N, E, f, d, G, E_0)$, where

- $N = \{x_1, x_2, x_3\}$,
- $E = \{e_1, e_2, e_3, e_4\}$,
- function f is defined such that

$$\begin{aligned} f(e_1) &= \{x_1, x_2\}, \\ f(e_2) &= \{x_2, x_3\}, \\ f(e_3) &= \{x_3, x_1\} & f(e_4) &= \{x_2, x_3\}, \end{aligned}$$

- function d is defined such that

$$\begin{aligned} d(e_1) &= \{x_1\} \rightarrow \{x_2\}, \\ d(e_2) &= \{x_2\} \rightarrow \{x_3\}, \\ d(e_3) &= \{x_3\} \rightarrow \{x_1\} & d(e_4) &= \{x_2\} \rightarrow \{\}, \end{aligned}$$

- underlying graph is shown in Figure 10 part b).
- $E_0 = \{e_1\}$

5 Hypergraph Automata for Picture Languages

In this section, we establish a strong connection between (WTS-)recognizable picture languages and picture graph languages that can be accepted by SA-hypergraph automata. We prove that the self-assembly of a Wang Tile System can be simulated by an SA-hypergraph automaton, see Theorem 1. The main idea is to start the tiling in the top left corner of a tiled picture and then extend the tiled picture downwards and rightwards, just as in Figure 3. Our converse result is slightly weaker: the picture language $L = p(\mathcal{L}(A))$, associated to the graph language accepted by an SA-hypergraph automaton A , is WTS-recognizable if A does not contain a *strong loop*, see Theorem 2. The restriction for A not to contain a strong loop is a natural assumption as strong loops cannot be used in any derivation that accepts a picture graphs.

Theorem 1. *For any recognizable picture language L there is a SA-hypergraph automaton A such that the picture language associated to the graph language $\mathcal{L}(A)$ is L .*

Proof. Let $V = (\Sigma, C', \Theta')$ be a Wang Tile System that recognizes the picture language L , that is $L = \mathcal{L}(V)$. We will slightly modify the WTS V such that it fulfils a certain property as described in the following. We define a WTS $W = (\Sigma, C, \Theta)$ which recognizes L and such that any two copies of a tile $t \in \Theta$ in a tiling of W must have a row- and a column-distance which is a multiple of 3. More precisely, for a Wang tiled version \bar{p} of a picture $p \in \mathcal{L}(W)$ where a tile $t \in \Theta$ appears at two positions $t = \bar{p}_{(i,j)} = \bar{p}_{(i',j')}$, we have that 3 divides $|i - i'|$

as well as $|j - j'|$. This is achieved by using 9 copies of every tile from V in W ; we let $\Theta = \Theta' \times \{0, 1, 2\} \times \{0, 1, 2\}$. We will ensure that a tile $(t, i, j) \in \Theta$ can only appear at position (i', j') if $i = i' \bmod 3$ and $j = j' \bmod 3$. This property is achieved by defining the glues as $C = C' \times \{0, 1, 2\}$, and for $t = (s, i, j) \in \Theta' \times \{0, 1, 2\} \times \{0, 1, 2\}$ we let

$$\begin{aligned} \lambda(t) &= \lambda(s), & \sigma_S(t) &= (\sigma_S(s), i), & \sigma_N(t) &= (\sigma_N(s), (i - 1) \bmod 3), \\ \sigma_E(t) &= (\sigma_E(s), j), & \sigma_W(t) &= (\sigma_W(s), (j - 1) \bmod 3). \end{aligned}$$

Note that a tiled picture \bar{p} of W can be converted into a tiled picture \bar{q} of V such that the corresponding pictures p and q coincide by applying the mapping $(t, i, j) \mapsto t$ to every tile in \bar{p} . Vice versa, a tiled picture \bar{q} in V can be converted into a tiled picture \bar{p} in W such that the corresponding pictures p and q coincide by applying the mapping $\bar{p}_{(i,j)} \mapsto (p_{(i,j)}, i \bmod 3, j \bmod 3)$ to every position in \bar{p} .

The modification of V will become of importance later in the proof: We need to ensure that for a 2×2 square of matching tiles t_1, t_2, t_3, t_4 , it is not possible to directly attach another copy of any of t_1, t_2, t_3, t_4 to this square.

We will define a SA-hypergraph automaton $A = (N, E, f, d, G, E_0)$ which simulates the assembly of a tiled picture from $L = \mathcal{L}(W)$ as described in Figure 3.

Let N be a set of nodes such that $|N| = |\Theta|$ and let $\vartheta: N \rightarrow \Theta$ be a bijection. For each node $x \in N$ there is a *corresponding tile* $\vartheta(x)$ and vice versa. Let N_T, N_R, N_B, N_L be the set of nodes which correspond to tiles on the top, right, bottom, left border of a tiled picture, respectively:

$$\begin{aligned} N_T &= \{x \in N \mid \sigma_N(\vartheta(x)) = \#\}, & N_R &= \{x \in N \mid \sigma_E(\vartheta(x)) = \#\}, \\ N_B &= \{x \in N \mid \sigma_S(\vartheta(x)) = \#\}, & N_L &= \{x \in N \mid \sigma_W(\vartheta(x)) = \#\}. \end{aligned}$$

Let $G = (N, E_v \cup E_h, \pi)$ be the underlying graph of A . The label function π is naturally defined as $\pi(x) = \lambda(\vartheta(x))$ for $x \in N$. For all nodes $x, y \in N$ there is an edge $(x, y) \in E_h$ if and only if $\sigma_E(\vartheta(x)) = \sigma_W(\vartheta(y)) \neq \#$ and either $x, y \in N \setminus (N_T \cup N_B)$ or $x, y \in N_T$ or $x, y \in N_B$; there is an edge $(x, y) \in E_v$ if and only if $\sigma_S(\vartheta(x)) = \sigma_N(\vartheta(y)) \neq \#$ and either $x, y \in N \setminus (N_L \cup N_R)$ or $x, y \in N_L$ or $x, y \in N_R$. This means if the east edge of a tile t can attach to the west edge of tile s , then their corresponding nodes $x = \vartheta^{-1}(t)$ and $y = \vartheta^{-1}(s)$ are connected by an h -edge $(x, y) \in E_h$. Analogously, if the south edge of a tile t can attach to the north edge of tile s , then their corresponding nodes $x = \vartheta^{-1}(t)$ and $y = \vartheta^{-1}(s)$ are connected by an v -edge $(x, y) \in E_v$.

If $N_T \cap N_B \neq \emptyset$ or $N_R \cap N_L \neq \emptyset$, the language $\mathcal{L}(W)$ possibly contains pictures p with $h(p) = 1$ or $w(p) = 1$, respectively, which can be seen as one-dimensional pictures. These pictures have to be treated separately. For now we assume that $N_T \cap N_B = N_R \cap N_L = \emptyset$.

The hyperedges E and the transition function d define the possible transitions of A . In every transition we add exactly one node to the graph of a configuration of A . Our naming convention is that x is the node which is attached in the derivation step and y, y_1, y_2, y_3 are incoming active nodes of the hyperedge. Every

graph containing only one node which corresponds to a tile in the top left corner is an initial graph. In order to construct a picture graph which represents a picture in $\mathcal{L}(W)$ we introduce three types of transitions, see Figure 11. The transitions of type I generate the top row of the graph and transitions of type II generate the left column of the graph; both transition types keep every generated node active. Transitions of type III generate the rest of the graph: A node is attached if it has a matching east neighbour (y_1), a matching north neighbour (y_3), and these two nodes are connected by another node (y_2); unless we reach the right or bottom border of the graph the nodes x , y_1 , and y_3 are active after using the transition.

Type	Hyperedges
I	$y \circ \xrightarrow{h} \bullet x$
II	$\begin{array}{c} y \\ \circ \\ \downarrow v \\ \bullet x \end{array}$
III	$\begin{array}{ccc} y_2 & \xrightarrow{h} & y_3 \\ \circ & & \circ \\ \downarrow v & & \downarrow v \\ y_1 & \xrightarrow{h} & \bullet x \end{array}$

Fig. 11. The hyperedges in the SA-hypergraph automaton A induce three different types of graphs. White nodes represent incoming active nodes of the hyperedges.

Formally, we define the set of hyperedges E , the set of initial edges E_0 , the function f , and the transition function d as following:

Initial graphs: For each $x \in N_T \cap N_L$, corresponding to a tile in the top left corner, we define a hyperedge $e_x \in E_0 \subseteq E$ with associated nodes $f(e_x) = \{x\}$ and the transition function $d(e_x) = \emptyset \rightarrow \{x\}$.

Type I: For all nodes $x, y \in N_T$, in the top row, such that $(x, y) \in E_h$, we define a hyperedge $e_{x,y} \in E$ with associated nodes $f(e_{x,y}) = \{x, y\}$ and the derivation function $d(e_{x,y}) = \{y\} \rightarrow \{x, y\}$.

Type II: For all nodes $x, y \in N_L$, in the left column, such that $(x, y) \in E_v$, we define a hyperedge $e_{x,y} \in E$ with associated nodes $f(e_{x,y}) = \{x, y\}$ and the derivation function $d(e_{x,y}) = \{y\} \rightarrow \{x, y\}$.

Type III: For all nodes $x \in N \setminus (N_T \cup N_L)$ and $y_1, y_2, y_3 \in N$ such that $(y_2, y_1), (y_3, x) \in E_v$ and $(y_2, y_3), (y_1, x) \in E_h$, we define a hyperedge $e_{x,y_1,y_2,y_3} \in E$ with associated nodes $f(e_{x,y_1,y_2,y_3}) = \{x, y_1, y_2, y_3\}$ and the derivation function

1. $d(e_{x,y_1,y_2,y_3}) = \{y_1, y_2, y_3\} \rightarrow \emptyset$ if $x \in N_B \cap N_R$, (bottom right corner)

2. $d(e_{x,y_1,y_2,y_3}) = \{y_1, y_2, y_3\} \rightarrow \{x, y_3\}$ if $x \in N_B \setminus N_R$, (bottom row)
3. $d(e_{x,y_1,y_2,y_3}) = \{y_1, y_2, y_3\} \rightarrow \{x, y_2\}$ if $x \in N_R \setminus N_B$, (right column)
4. $d(e_{x,y_1,y_2,y_3}) = \{y_1, y_2, y_3\} \rightarrow \{x, y_2, y_3\}$ otherwise.

Consider the graph G_e which is induced by the hyperedge $e \in E$. Depending on the type of the hyperedge e , the graph G_e contains at least the edges shown in Figure 11. However, by the modification of the Wang tile system V above, we ensured that the graph G_e contains exactly those edges shown in Figure 11. Suppose one of the graphs G_e would contain an edge (x', y') which is not shown in Figure 11, then the tile corresponding to y' could occur in two positions which are less than three rows and columns apart — a property that was excluded by the modification.

We will show that $p(\mathcal{L}(A)) = L$. Firstly, consider an array \bar{p} of tiles from Θ which is the Wang-tiled version of the picture $p \in \mathcal{L}(W)$. We will show that the SA-hypergraph automaton A accepts a picture graph M such that $p(M) = p$. We assume M to be embedded in \mathbb{Z}^2 such that the nodes cover the axis-parallel rectangle spanned by the points $(1, 1)$ and $(h(p), w(p))$, every v -edge points downwards, and every h -edge points rightwards; recall that our coordinates represent the rows and columns of a matrix. The derivation leading to the final configuration (M, \emptyset, g) simulates the assembly of tiles which form \bar{p} as shown in Figure 3. The north and west edges of the tile $t_{TL} = \bar{p}_{(1,1)}$ in the top left corner of \bar{p} are labelled by $\#$, and therefore, the node $x_{TL} = \vartheta^{-1}(t_{TL})$ corresponding to t_{TL} forms an initial graph M_0 . The adjacent edges of two neighbouring tiles s, t in \bar{p} are labelled by the same colour. Suppose s is the west neighbour of t , then $\sigma_E(s) = \sigma_W(t) \neq \#$ and both tiles belong to the same row, implying that $\sigma_N(s) = \# \iff \sigma_N(t) = \#$ and $\sigma_S(s) = \# \iff \sigma_S(t) = \#$. Therefore, their corresponding nodes in G are connected by an h -edge $(\vartheta^{-1}(s), \vartheta^{-1}(t)) \in E_h$. Analogously, if s is the north neighbour of t , then $(\vartheta^{-1}(s), \vartheta^{-1}(t)) \in E_v$. Next, we see that the hyperedges of type I and type II can be used in order to create the top row and left column of the graph M , respectively. Furthermore, the hyperedges of type III can be used in order to create all the remaining nodes of M . We conclude that $(M_0, \{x_{TL}\}, id) \xrightarrow{*}_A (M, O, g)$ is a derivation in A and we will prove that (M, O, g) has to be a final configuration with $O = \emptyset$. Observe, that hyperedges of types I and II leave all the nodes active while hyperedges of type III deactivate at least the top left node in the hyperedge. Thus, all nodes except for those in the bottom row and in the right column will be deactivated in the configuration (M, O, g) . Furthermore, in order to create the bottom row and right column hyperedges of type III.2 and III.3 are used, respectively, and one rule of type III.1 is used in order to create the bottom-right node of M . It is easy to see that the derivation function is designed such that all nodes will be deactivated in the configuration (M, O, g) and, therefore, A accepts M .

Now, let $M = (N_M, E_{v,M} \cup E_{h,M}, \pi_M) \in L(A)$ be a graph which is generated by A . Let G be accepted by the derivation

$$(M_0, O_0, g_0) \xrightarrow{A} (M_1, O_1, g_1) \xrightarrow{A} \cdots \xrightarrow{A} (M_k, O_k, g_k)$$

where $(M_0, O_0, g_0) = (G_{e_0}, O_{e_0}, id)$ is an initial configuration with $e_0 \in E_0$ and $(M_k, O_k, g_k) = (M, \emptyset, g)$ is a final configuration. Let N_i be the node set of the graph M_i . Note that for any $0 \leq i \leq k$ the function g_i is the restriction of g by N_i , that is $g_i = g|_{N_i}$. In order to avoid confusion, nodes in the graph M are consistently denoted by x, y and nodes in the graph G are consistently denoted by x', y' ; the nodes may have subscripts.

Let the nodes in the graphs M_0, \dots, M_k be embedded in \mathbb{Z}^2 such that all h -edges point rightwards and all v -edges point downwards; just like we did above. The creation of graph $M = M_k$ starts with the initial graph M_0 which contains only one node $x_{TL} \in N_T \cap N_L$. Let x_{TL} lie on position $(1, 1)$ in all of the graphs M_0, \dots, M_k . The graph M_0 can be extended rightwards by using hyperedges of type I and downwards by hyperedges of type II. Since none of the hyperedges attach a new node upwards or leftwards of an existing node in M_{i-1} in order to obtain M_i , the node x_{TL} lies in the top row and in the left column of M_i . By the definition of type I and II hyperedges, for every node y in the top row (resp., left column) of M we have $g(y) \in N_T$ (resp., $g(y) \in N_L$). By using hyperedges of type III the area spanned by the top row and left column can be filled with nodes. It is easy to see that for all graphs M_0, \dots, M_k we have that if a node lies on position (i, j) , then for all $(i', j') \in [i] \times [j]$ a node lies on position (i', j') . Furthermore, if $i' < i$, then the node on position (i', j') has an outgoing v -edge, and if $j' < j$, then the node on position (i', j') has an outgoing h -edge. In other words, in the axis-parallel rectangle spanned by the points $(1, 1)$ and (i, j) all nodes are connected by edges with all direct neighbours (nodes which have an Euclidean distance of 1).

In the final configuration (M_k, \emptyset, g) there is no active node. Thus, the last node which is added to the graph M_{k-1} in order to obtain M_k is a node x_{BR} such that $g(x_{BR}) \in N_B \cap N_R$, as all other derivation rules will leave some nodes active. Next, let us consider the nodes which belong to the same row and column as x_{BR} does. Note that if two nodes x and y in M are connected by an edge, then the corresponding nodes $g(x)$ and $g(y)$ in G are connected by an edge, too; more precisely, if $(x, y) \in E_{v,M}$, then $(g(x), g(y)) \in E_v$, and if $(x, y) \in E_{h,M}$, then $(g(x), g(y)) \in E_h$. Since a node in N_B (resp., N_R) only is connected by h -edges (resp., v -edges) in G to other nodes from N_B (resp., N_R), we see that for every node y in the row of x_{BR} (resp., column of x_{BR}) we have $g(y) \in N_B$ (resp., $g(y) \in N_R$). A node $y' \in N_B$ (resp., $y' \in N_R$) does not have any outgoing v -edges (resp., h -edges) as the south edge (resp., east edge) of $\vartheta(y')$ is labelled by $\#$. We conclude that x_{BR} sits in the bottom row and right column of the graph M and, by the observations made above, this implies that M is a picture graph.

We claim that the picture $p(M)$ which corresponds to the graph M can be generated by the assembly \bar{p} given by the embedding of nodes in M and the function $\vartheta \circ g$. Clearly, for every node y on position (i, j) in M we have that $p(M)_{i,j} = \pi_M(y) = \lambda(\vartheta(g(y)))$, therefore, the pictures p and $\lambda(\bar{p})$ coincide. Next, we prove that \bar{p} is a tiled picture in the Wang tile system W . Recall, that all nodes on the top, right, bottom, and left border of M correspond to tiles in

M_T , M_R , M_B , and M_L , respectively, and therefore, \bar{p} is well-bordered. Let t_x and t_y be two neighbouring tiles in \bar{p} which lie on positions (i, j) and $(i, j + 1)$, respectively. Let x and y be the nodes in M which lie on the positions (i, j) and $(i, j + 1)$, respectively. Note that $t_x = \vartheta(g(x))$ and $t_y = \vartheta(g(y))$. Since M is a picture graph, $(x, y) \in E_{h,M}$ and $(g(x), g(y)) \in E_h$. The edge set E_h was build to ensure that $\sigma_E(t_x) = \sigma_W(t_y)$. We conclude that all adjacent east-west edges in \bar{p} have matching colours. By symmetric arguments, we also conclude that all adjacent north-south edges in \bar{p} have matching colours. Therefore, \bar{p} is a tiled picture in W and $p \in L$.

Finally, let us consider the case when $N_T \cap N_B \neq \emptyset$. We can add a component to the SA-hypergraph automaton which works similar to a non-deterministic finite automaton and where every hyperedge induces an graph of type I in Figure 11. The initial graphs are given by all nodes from $N_T \cap N_B \cap N_L$. For all nodes $x, y \in N_T \cap N_B$ with $(y, x) \in E_h$ we define a hyperedge $e_{x,y}$ such that $f(e_{x,y}) = \{x, y\}$. The derivation function is given as $d(e_{x,y}) = \{y\} \rightarrow \{x\}$ if $x \notin N_R$, and $d(e_{x,y}) = \{y\} \rightarrow \emptyset$ otherwise. Obviously, this attachment to the hypergraph A accepts all graphs which correspond to pictures $p \in L$ with $h(p) = 1$. The case when $N_L \cap N_R \neq \emptyset$ can be covered analogously. \square

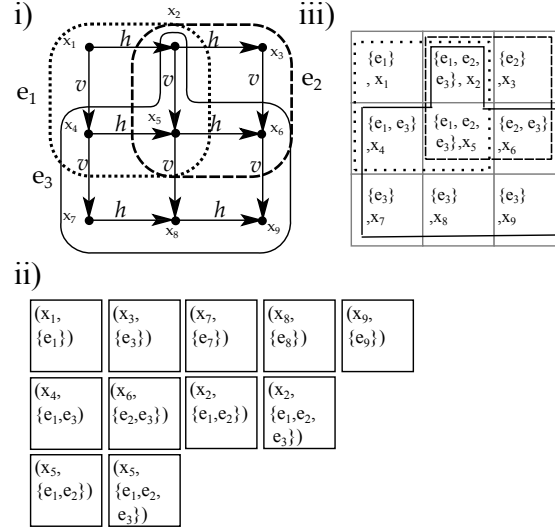


Fig. 12. Let $A = (N, E, f, d, G, E_0)$ be a SA-hypergraph automaton where N , E , f , and G are defined in part i). function d is defined such that $d(e_1) = \{x_1\} \rightarrow \{x_2, x_4, x_5\}$, $d(e_2) = \{x_2, x_5\} \rightarrow \{x_2, x_5, x_6\}$ and $d(e_3) = \{x_2, x_4, x_5, x_6\} \rightarrow \{\}$. SA-hypergraph automaton starts from e_1 . Part ii) shows the set of all the possible tile candidates. On each tile related node and the set of ψ are written. The tiling on part iii) is the result of overlapping of three hyperedges e_1, e_2 and e_3 .

Next, we prove that a picture language $L = p(\mathcal{L}(A))$, associated to the graph language $\mathcal{L}(A)$, is WTS-recognizable if A does not contain a strong loop.

Let A be an SA-hypergraph automaton. A series of hyperedges $s = \langle e_0, e_1, \dots, e_n \rangle$ from A is a (*derivation*) *loop* if $e_0 = e_n$ and $Q_{2,i} \cap Q_{1,i+1} \neq \emptyset$ where $d(e_i) = Q_{1,i} \rightarrow Q_{2,i}$ for $0 \leq i < n$. Loops in an SA-hypergraph automaton are a prerequisite for using a hyperedge several times in one derivation. Therefore, an SA-hypergraph automaton without any loops can only accept a finite graph language. Let $G_i = G_{e_i}$ be the graph induced by e_i , let x be a node in $G_0 = G_n$, and let $O_i = Q_{2,i} \cap Q_{1,i+1}$ be set overlapping incoming/outgoing active nodes of G_i and G_{i+1} . There is a path in the underlying graph of A from x to x which only visits the subgraphs G_0, \dots, G_n , in the given order, and passes through at least one node of each O_i (the path may use incoming and outgoing edges). The loop s is a *strong loop* if, on this path, the number of incoming horizontal edges equals the number of outgoing horizontal edges and the number of incoming vertical edges equals the number of outgoing vertical edges. In other words, when starting from a configuration M and successively gluing the hyperedges from s to M , then the subgraph added by the hyperedge e_0 and the subgraph added by the hyperedge e_n fully overlap when naturally embedded in \mathbb{Z}^2 . Note that, by Remark 1, all graphs G_i are subgrids which implies that the choice of the path from x to x does not matter in this definition.

Theorem 2. *Let A be a SA-hypergraph automaton without any strong loops. The picture language $L = p(\mathcal{L}(A))$, associated to the graph language $\mathcal{L}(A)$, is WTS-recognizable (Wang tile system recognizable).*

Proof. Let $A = (N, E, f, d, G, E_0)$ and let $G = (N, E_v \cup E_h, \pi)$. We may assume that $e \in E_0$ if and only if $d(e) = \emptyset \rightarrow O_e$. Therefore, none of the initial hyperedges can be used in a transition. This assumption is justified by the fact that we can duplicate all hyperedges in E_0 such that one copy can be used in a transition but does not belong to E_0 and the other copy which belongs to E_0 cannot be used in a transition. Furthermore, any hyperedge without incoming active nodes which does not belong to E_0 is useless and can be removed from E .

For a node $x \in N$ we define the list of *related hyperedges* to x , $H_x = \{e \in E \mid x \in f(e)\}$. Let x be a node and $\psi \subseteq H_x$. We call a hyperedge $g \in \psi$ a *generator* of (x, ψ) if $x \notin Q_1$ with $d(g) = Q_1 \rightarrow Q_2$. Note that if $g \in E_0$, then g must be a generator. We call a hyperedge $c \in \psi$ a *consumer* of (x, ψ) if $x \notin Q_2$ with $d(c) = Q_1 \rightarrow Q_2$. The pair (x, ψ) is a *tile candidate* if ψ contains exactly one generator $g_{(x, \psi)}$ and exactly one consumer $c_{(x, \psi)}$; furthermore, if $g_{(x, \psi)} = c_{(x, \psi)}$, we require that $\psi = \{g_{(x, \psi)}\}$. Note that if $g_{(x, \psi)} \neq c_{(x, \psi)}$, then for all $e \in \psi$ with $d(e) = Q_1 \rightarrow Q_2$, we have that $x \in Q_1$ unless e is the generator and $x \in Q_2$ unless e is the consumer. The tile candidate (x, ψ) describes the attachment of a copy of the node x to the output graph by the generator; afterwards, x is used as active node by all hyperedges in $\psi \setminus \{g_{(x, \psi)}, c_{(x, \psi)}\}$; finally, x is deactivated by the consumer. Let G_ψ be the node-induced subgraph of G by $\bigcup_{e \in \psi} f(e)$. If G_ψ is not a subgrid (a subgraph of some picture graph), we remove (x, ψ) from the set of tile candidates. Let Ψ denote the set of all remaining tile candidates.

The Wang tile system $W = (\Sigma, C, \Theta)$ which recognizes L is constructed based on the list Ψ . In order to recognize the picture language associated to $\mathcal{L}(A)$, we have to define the attachments of tile candidates. We use unordered pairs $\{(x, \psi), (y, \varphi)\} \in \Psi^2$ of tile candidates for the colours on the edges. For a tile candidate $(x, \psi) \in \Psi$ we define the set of labelled Wang tiles

$$\Theta_{(x, \psi)} = \mathcal{S}_{N, (x, \psi)} \times \mathcal{S}_{E, (x, \psi)} \times \mathcal{S}_{S, (x, \psi)} \times \mathcal{S}_{W, (x, \psi)} \times \{l_x\}$$

where l_x is the label $\pi(x)$ and $\mathcal{S}_{N, (x, \psi)}$, $\mathcal{S}_{E, (x, \psi)}$, $\mathcal{S}_{S, (x, \psi)}$, $\mathcal{S}_{W, (x, \psi)}$ are sets of colours which are defined below. The set of all tiles is the union $\Theta = \bigcup_{(x, \psi) \in \Psi} \Theta_{(x, \psi)}$.

For $(x, \psi), (y, \varphi) \in \Psi$, we let $\{(x, \psi), (y, \varphi)\} \in \mathcal{S}_{E, (x, \psi)}$ and $\{(x, \psi), (y, \varphi)\} \in \mathcal{S}_{W, (y, \varphi)}$ if and only if

1. $(x, y) \in E_h$,
2. $H_x \cap \varphi \subseteq \psi$,
3. $\psi \cap H_y \subseteq \varphi$, and
4. $g_{(x, \psi)} = g_{(y, \varphi)}$ or $y \in Q_1$ for $d(g_{(x, \psi)}) = Q_1 \rightarrow Q_2$ or $x \in Q'_1$ for $d(g_{(y, \varphi)}) = Q'_1 \rightarrow Q'_2$.

For $(x, \psi), (y, \varphi) \in \Psi$, we let $\{(x, \psi), (y, \varphi)\} \in \mathcal{S}_{S, (x, \psi)}$ and $\{(x, \psi), (y, \varphi)\} \in \mathcal{S}_{N, (y, \varphi)}$ if and only if $(x, y) \in E_v$ and conditions 2 to 4 are satisfied. For $(x, \psi) \in \Psi$, we let $\mathcal{S}_{E, (x, \psi)} = \{\#\}$ if x does not have an incoming vertical edges in the graph G_ψ . By symmetric condition we let $\mathcal{S}_{N, (x, \psi)} = \{\#\}$, $\mathcal{S}_{S, (x, \psi)} = \{\#\}$, or $\mathcal{S}_{W, (x, \psi)} = \{\#\}$.

Now, consider an $m \times n$ -picture graph $M = (N_M, E_{v, M} \cup E_{h, M}, \pi_M) \in \mathcal{L}(A)$. We will show that there is a tiled version \bar{p} of picture $p = p(M)$ which uses tiles from Θ and, therefore, p is recognized by W . Let G be accepted by the derivation

$$(M_0, O_0, g_0) \xrightarrow{A} (M_1, O_1, g_1) \xrightarrow{A} \cdots \xrightarrow{A} (M_k, O_k, g_k)$$

where $(M_0, O_0, g_0) = (G_{e_0}, O_{e_0}, id)$ is an initial configuration (that is $e_0 \in E_0$) and $(M_k, O_k, g_k) = (M, \emptyset, g)$ is a final configuration. Let e_i be the hyperedge and $P_i \subseteq O_{i-1}$ be the active nodes which are used in the transition $(M_{i-1}, O_{i-1}, g_{i-1}) \xrightarrow{A} (M_i, O_i, g_i)$. Let $d(e_i) = Q_{1,i} \rightarrow Q_{2,i}$ for $1 \leq i \leq k$. Recall that, by definition, M_{i-1} is a full subgraph of M_i and, by induction, every graph M_i is a full subgraph of M . Being an $m \times n$ -picture graph, the nodes in M can be naturally embedded in $[m] \times [n]$ by the function f_M .

Consider one node $x' \in N_M$ and its original $x = g(x')$ in G . We assign to x' a list of hyperedges $\psi \subseteq E$ such that $e_i \in \psi$ if $x' \in P_i$ or x' belongs to M_i but not M_{i-1} . We intend to use a tile from $\Theta_{(x, \psi)}$ for the pixel $\bar{p}_{f_M(x')}$ representing x' in the tiled picture \bar{p} . Observe that ψ contains a consumer as x' is not active in the final configuration and ψ cannot contain two consumers because a node can only be deactivated once. In addition, the hyperedge e_i such that x' belongs to M_i but not M_{i-1} is the single generator in ψ . Since G_ψ is isomorphic to a subgraph of M , we conclude that (x, ψ) is indeed a tile candidate. If x' does not have an outgoing horizontal edge, then the node x in the graph G_ψ cannot have an outgoing horizontal edge either and, therefore, $\mathcal{S}_{E, (x, \psi)} = \{\#\}$. Symmetric

arguments apply if x does not have an incoming horizontal, outgoing vertical, or incoming vertical edge.

Next, consider two nodes $x', y' \in N_M$ which are connected by an edge and, by symmetry, assume (x', y') is a horizontal edge. Let $x = g(x')$, $y = g(y')$ be their originals and let ψ, φ be the set of hyperedges associated to x', y' , respectively. We will show that $\{(x, \psi), (y, \varphi)\}$ is a colour in $\mathcal{S}_{E, (x, \psi)}$ as well as in $\mathcal{S}_{W, (y, \varphi)}$. Thus, we can choose tiles from $\Theta_{(x, \psi)}$ and $\Theta_{(y, \varphi)}$ for the positions $f_M(x')$ and $f_M(y')$ in \bar{p} , respectively. Clearly, the choice of the tiles also depends on the other neighbours of x' and y' . We have to show that conditions 1 to 5, above, are satisfied. The first condition is satisfied by assumption. By contradiction, suppose the second condition is not satisfied. There is $e_i \in H_x \cap \varphi \setminus \psi$; thus, in the i -th step of the derivation we use the hyperedge e_i that presupposes or generates an edge (x'', y') in M where $g(x'') = x$ but $x'' \neq x'$. This would imply that y has two incoming horizontal edges whence M is not a picture graph. The third condition is satisfied by symmetric arguments. The edge (x', y') in M can only be created in a step i where x' or y' is added to the graph M_{i-1} . Thus, x' and y' either have the same generator in (x, ψ) and (y, φ) , or x' is in the active nodes when y' is generated, or y' is in the active nodes when x' is generated. In all cases condition 4 is satisfied.

We conclude that a tiled picture \bar{p} such that $p = p(M)$ and $M \in \mathcal{L}(A)$ can be generated by using tiles from Θ and, therefore, $p(M) \in \mathcal{L}(W)$.

Consider a picture $p \in \mathcal{L}(W)$ and let \bar{p} be the tiled version of p , using tiles from $\Theta = \bigcup_{(x, \psi) \in \Psi} \Theta_{(x, \psi)}$.

We start by introducing the concept of masks which can be seen as connected subpictures of the tiled picture \bar{p} that represent the nodes in one hyperedge. A *mask* \mathbf{m} is a $h(\bar{p}) \times w(\bar{p})$ matrix of tiles from $\Theta \cup \{\text{empty}\}$, such that either $\mathbf{m}_{(i, j)} = \text{empty}$ or $\mathbf{m}_{(i, j)} = \bar{p}_{(i, j)}$ for all $(i, j) \in [h(\bar{p})] \times [w(\bar{p})]$. In addition, we require that the non-empty entries in \mathbf{m} are connected; that is, for every pair of tiles $\mathbf{m}_{(i', j')}, \mathbf{m}_{(i, j)} \in \Theta$ there exists a sequence $r = \langle r_0, r_1, \dots, r_n \rangle$ of tiles in \mathbf{m} such that $r_0 = \mathbf{m}_{(i, j)}$, $r_n = \mathbf{m}_{(i', j')}$, $r_k \in \Theta$, and r_k, r_{k+1} must be adjacent for all $0 \leq k < n$.

Let $e \in E$ be an hyperedge and let $G_e = (N_e, E_{e,v} \cup E_{e,h}, \pi_e)$ be the graph induced by this hyperedge. By Remark 1, we assume that G_e is a subgrid. We say G_e is mapped to a mask \mathbf{m} if there is a injective function $h: N_e \rightarrow [h(\bar{p})] \times [w(\bar{p})]$ which satisfies: $\mathbf{m}_{(i, j)}$ belongs to Θ if and only if (i, j) is in the domain of h ; for all nodes $x, y \in N_e$ there is an edge $(x, y) \in E_{e,h}$ (resp., $(x, y) \in E_{e,v}$) if and only if $h(x)$ is in north (resp., west) neighbour of $h(y)$. Whenever we use this mapping, we will ensure that for all $x \in G_e$ the tile $\bar{p}_{h(x)}$ belongs to $\Theta_{(x, \psi)}$ for some $\psi \subseteq E$.

Consider a tile $t \in \bar{p}_{(i, j)} \in \Theta_{(x, \psi)}$ and a hyperedge $e \in \psi$. We define the mask $\mathbf{m}^{[(i, j), x, e]}$ such that the graph G_e can be mapped by function h to $\mathbf{m}^{[(i, j), x, e]}$ and $h(x) = (i, j)$. We say that e is the hyperedge related to the mask $\mathbf{m}^{[(i, j), x, e]}$. Let $t' = \bar{p}_{(i', j')} \in \Theta_{(y, \varphi)}$ be a tile that is adjacent to t and let $e \in \psi$. For simplicity we only consider the case when t' is the east neighbour of t ; i.e., $(i', j') = (i + 1, j)$. We will show that if (i', j') is non-empty in $\mathbf{m}^{[(i, j), x, e]}$, then

$e \in \varphi$. Since t' is the east neighbour of t conditions 1 to 4, above, apply. As (i', j') is non-empty in $\mathbf{m}^{[(i,j),x,e]}$, there exists a horizontal edge (x, z) in G_e . Furthermore, from conditions 1 and 4 it follows that (x, y) is a horizontal edge in the graph G_g induced by the generator $g = g_{(x,\varphi)}$. As both graphs G_e and G_g are subgraphs of the subgrid G_ψ , we see that the edges (x, y) and (x, z) coincide, thus, $y = z$. We conclude $y \in G_e$ and $e \in H_y$. By condition 3, $e \in \varphi$. Because the hyperedge e induces a connected graph, we can infer that for all non-empty $\mathbf{m}_{(i'',j'')}^{[(i,j),x,e]} \in \Theta_{(z,\chi)}$, we find $e \in \chi$. Note that this also implies that $\mathbf{m}^{[(i,j),x,e]} = \mathbf{m}^{[(i',j'),y,e]} = \mathbf{m}^{[(i'',j''),z,e]}$.

We define the set of masks $\mu = \{\mathbf{m}^{[(i,j),x,e]} | \bar{p}_{(i,j)} \in \Theta_{(x,\psi)}, e \in \psi\}$ which are induced by hyperedges in the above manner. Intuitively, every mask in μ represents one transition in the derivation of a picture graph M which represents the picture $p = p(M)$. In order to use a transition defined by a mask, we need to guarantee that all of its input areas exist and are active. We will order the set μ accordingly. Let us define the relation $R \subseteq \mu \times \mu$ such that $(\mathbf{m}, \mathbf{n}) \in R$ if the transition represented by \mathbf{m} has to be used before the transition represented by \mathbf{n} . Let \mathbf{m} and \mathbf{n} be two distinct masks in μ . The pair (\mathbf{m}, \mathbf{n}) is in R if there exists (i, j) such that $\mathbf{m}_{(i,j)} = \mathbf{n}_{(i,j)} \in \Theta_{(x,\psi)}$, and $\mathbf{m} = \mathbf{m}^{[(i,j),x,g]}$ where $g = g_{(x,\psi)}$ or $\mathbf{n} = \mathbf{m}^{[(i,j),x,c]}$ where $c = c_{(x,\psi)}$. The pair (μ, R) can be seen as directed graph G_μ . First, we show that the graph G_μ does not contain any loops, afterwards, a topological sort of this graph is used to order the transitions represented by the masks.

When two or masks overlap on a tile (have a common non-empty entry), regarding the construction of tile candidates, we know that the related hyperedge of exactly one of these masks is the generator of the input area of the other hyperedges. Hence, these masks are connected in the graph G_μ . By contradiction, assume that $\langle \mathbf{n}_0, \mathbf{n}_1, \dots, \mathbf{n}_l \rangle$ is a non-trivial loop in G_μ (i.e., $(\mathbf{n}_i, \mathbf{n}_{i+1}) \in R$ for every $0 \leq i < l-1$ and $(\mathbf{n}_l, \mathbf{n}_0) \in R$). However, the sequence of related hyperedges to this sequence of mask is a strong loop in the SA-hypergraph automaton A which was excluded by assumption. Moreover, since two tiles with different generators cannot connect without satisfying conditions 4, the graph G_μ must be connected. Therefore, graph G_μ can be topologically sorted. Sorting of the hyperedges guaranteed that the active input nodes of one hyperedge are generated before the gluing of the hyperedge.

By contraction, assume that graph G_μ has two distinct nodes \mathbf{m}_1 and \mathbf{m}_2 without any input edges. Let \mathbf{m}_3 be the first node in the topological order such that paths $\mathbf{m}_1 \rightarrow^* \mathbf{m}_3$ and $\mathbf{m}_2 \rightarrow^* \mathbf{m}_3$ exist in G_μ . As \mathbf{m}_3 is chosen minimal, these paths do not share any node other than \mathbf{m}_3 . Recall that all incoming active nodes of a hyperedge are connected. Considering that two nodes cannot connect to each other unless they are in the same hyperedge or they have glued to each other, we have a contradiction as \mathbf{m}_3 cannot be the first common node on both paths. We conclude that graph G_μ has only one node without input.

Now, let $\mathbf{m}_0, \mathbf{m}_1, \dots, \mathbf{m}_k$ be the topological sort of μ by the relation \mathcal{R} . We define $\mathbf{m} + \mathbf{n} = \mathbf{o}$ such that $\mathbf{o}_{(i,j)} = \text{empty}$ if $\mathbf{m}_{(i,j)} = \mathbf{n}_{(i,j)} = \text{empty}$; otherwise,

$\mathfrak{o}_{(i,j)} = \bar{p}_{(i,j)}$. We will show that a graph M_k can be generated by a derivation

$$(M_0, O_0, g_0) \xrightarrow{A} (M_1, O_1, g_1) \xrightarrow{A} \cdots \xrightarrow{A} (M_k, O_k, g_k)$$

such that the graph M_i can be mapped to the mask $\sum_{j=0}^i \mathfrak{m}_j$; this implies that m_k can be mapped to $\bar{p} = \sum_{j=0}^k \mathfrak{m}_j$. Let e_i be the hyperedge related to the mask \mathfrak{m} . The graph $M_0 = G_{e_0}$ is an initial graph because \mathfrak{m}_0 has no incoming edges in \mathcal{G}_μ and, therefore, the derivation function of e_0 is $d(e_0) = \emptyset \rightarrow Q_2$; thus, (M_0, O_0, g_0) where $O_0 = Q_2$ and $g_0 = id$ is an initial configuration. In derivation step $(M_{i-1}, O_{i-1}, g_{i-1}) \xrightarrow{A} (M_i, O_i, g_i)$ we use the hyperedge e_i . By induction,

we can assume that M_{i-1} can be mapped to $\sum_{j=0}^{i-1} \mathfrak{m}_j$ by a function h_{i-1} . There is only one way to glue the hyperedge e_i to M_{i-1} such that resulting graph M_i can be mapped to $\sum_{j=0}^i \mathfrak{m}_j$. We have to prove that all incoming active nodes of G_{e_i} exist and are active in M_i . Let x be an incoming active node which is represented by the tile $\bar{p}_{(a,b)} \in \Theta_{(x,\psi)}$. The definition of R ensures that the mask representing the generator of (x, ψ) in (a, b) has already been used and that the mask representing the consumer of (x, ψ) in (a, b) has not yet been used. Finally, every tile candidate has a consumer which means that there are no active nodes in the final configuration (M_k, O_k, g_k) . As result, the picture p , generated by the suggested tiling system, is in $p(\mathcal{L}(A))$. \square

6 Conclusion

We introduced SA hypergraph automata, a language/automata theoretic model for patterned self-assembly systems. SA hypergraph automata accept all recognizable picture languages but, unlike other models, (e.g. Wang Tile Automata) SA-hypergraph automata do not rely on an *a priori* given scanning strategy of a picture. This property makes the SA hypergraph automata better suited to model DNA-tile-based self-assembly systems.

SA-hypergraph automata provide a natural automata-theoretic model for patterned self-assemblies that will enable us to analyse self-assembly in an automata-theoretic framework. This framework lends itself easily to, e.g., descriptive and computational complexity analysis, and such studies may ultimately lead to classifications and hierarchies of patterned self-assembly systems based on the properties of their corresponding SA-hypergraph automata. An additional feature is that each SA-hypergraph automaton accepts an entire class of “supertiles” as opposed to a singleton set, which may also be of interest for some applications or analyses.

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